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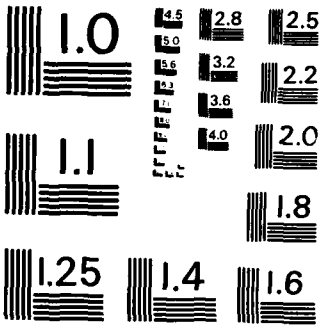

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)
Basic studies of photoionization processes in atoms and molecules have been carried out using triply differential (differential in incident wavelength, ejected electron energy, and ejection angle) photoelectron spectroscopy with synchrotron radiation as the excitation source. Measurements have been conducted in the vacuum ultraviolet wavelength range up to $h\nu \sim 35$ eV on a variety of atomic and molecular systems. Photoelectron branching ratios (partial photoionization cross sections) and photoelectron angular distribu-

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FINAL REPORT

TRIPLY DIFFERENTIAL STUDIES OF ATOMIC AND MOLECULAR PHOTOIONIZATION USING SYNCHROTRON RADIATION (Contract No. N00014-85-F-0016)

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I. SCIENTIFIC PROBLEM

The research supported by this contract involves basic studies of vacuum ultraviolet (VUV) photoionization processes in atoms and molecules. Using advanced experimental approaches, described in Section II, we seek to develop new insight and basic data concerning the spectroscopy and dynamics of atomic and molecular photoionization by observing complementary observables, e.g., partial photoionization cross sections, photoelectron branching ratios, and photoelectron angular distributions. These studies have led to novel measurements and to new insight into photoionization mechanisms, particularly regarding the effects of shape resonances and autoionization on vibrational ionization channels.

In addition to our prime goal of developing a clear understanding of photoionization spectroscopy and dynamics, this work impacts on at least three other areas: First, we seek to develop new probes of the photoionization process. In recent annual periods, this project has introduced the techniques of fluorescence polarization spectroscopy of molecules and photoelectron-photoion coincidence spectroscopy of clusters formed in a supersonic expansion. At the present time, attention is focussed on use of a new, high-resolution angle-resolved, dual photoelectron spectrometer system (discussed below). Future work will be aimed at such experiments as electron-electron coincidence studies, VUV photoionization of laser-excited states, and photoelectron-photoion coincidence studies of molecular fragmentation using synchrotron radiation. Second, this project produces data crucial for testing theoretical predictions and, thus, contributes to the development of realistic theories of atomic and molecular photoionization. Third, the data produced by this project contribute to characterizing the alternative pathways by which radiation interacts with matter, and hence contributes to the macroscopic modeling of such microscopic interactions.

II. SCIENTIFIC AND TECHNICAL APPROACH

The main experimental approach used in this work involves triply differential photoelectron measurements using synchrotron radiation as the continuously tunable source of ionizing radiation. By triply differential photoelectron studies, we mean that photoelectron intensity measurements are made as a function of three completely independent variables -- the incident wavelength, λ, the kinetic energy of the ejected electron, T, and the angle of ejection, θ, relative to the polarization direction of the light. Variation of λ permits the systematic mapping of photoionization properties throughout the vacuum-ultraviolet wavelength range, including probing important spectral features such as autoionizing states, shape resonances, and near-threshold phenomena. Variation of T permits the selection of particular electronic-vibrational-(rotational) states formed in the photoionization process. Hence, by monitoring the whole manifold of final states (different T's), one can determine the effect of alternative photoionization mechanisms (selected by choosing λ, as discussed above) on relative probabilities of forming the various final states. Variation of θ permits the characterization of the angular distribution of photoelectrons for each final state and λ. In photoionization of free atoms and molecules the angular dependence of photoelectron intensity has the simple form

$$\frac{d\sigma}{d\theta} = \frac{\sigma_{tot}}{4\pi}\left[1 + \beta P_2(\cos\theta)\right],$$

where σ_{tot} is the integrated cross section and β is called the asymmetry parameter. Therefore, the angular distribution as a function of (T,λ) can be characterized by β, which in turn can be measured by recording peak strengths at as little as two angles. While it is true that most applications of photoionization data hinge primarily on partial cross sections (or branching ratios), angular distributions play an indispensable role in testing theoretical models and in the fundamental understanding of the photoionization process. Hence, both branching ratios and β's are critical to sound scientific study of photoionization processes.

In addition, this project introduced two techniques to address new types of problems in molecular photoionization. These are fluorescence polarization spectroscopy of molecules and photoelectron-photoion coincidence spectroscopy on selected clusters formed in mixtures in supersonic expansions. Expertise in these techniques is available for use in future research as the need arises. Further development of our measurement capabilities is under consideration but is also subject to staffing levels. Experimental approaches of interest include electron-electron coincidence measurements of double electron ejection, VUV photoionization of laser excited states, and photoelectron-photoion coincidence studies of molecular fragmentation using synchrotron radiation.

III. WORK ACCOMPLISHED

The work accomplished during the 5 1/4 years of this project are reflected, in part, in the 36 papers, 36 abstracts of contributed talks, and 37 invited lectures listed in Section IV. In this section, we briefly describe the highlights of this body of work in eleven categories:

(1) This project pioneered the vibrationally-resolved study of the effects of autoionizing resonances on photoionization branching ratios and photoelectron angular distributions.

(2) This project pioneered the equivalent type of study on shape resonances, although two of the initial measurements were reported immediately prior to the beginning of this contract.

(3) This project produced important studies of shape resonance effects in large molecules, e.g., SF_6 and BF_3, in which detailed comparisons with recent calculations indicated the state-of-the-art in understanding the photoionization dynamics of large molecules, as well as points to be resolved in future experimental and theoretical work.

(4) This project was the first to investigate the effects of both shape resonances and autoionizing resonances in excitation of bending vibrations in polyatomic molecules. This will be a significant theme in future studies of molecular photoionization with synchrotron radiation.

(5) This project first introduced the technique of polarization of fluorescence to study the dynamics of molecular photoionization, including unique ability to measure such quantities as branching ratios between degenerate photoionization channels.

(6) This project produced a substantial amount of data on photoionization branching ratios and photoelectron angular distributions of a variety of molecules, including N_2, CO, NO, H_2, CO_2, C_2H_2, SO_2, HCN, C_2N_2, CH_3CH, BF_3, and SF_6.

(7) This project produced the first (and, as of yet, only) photoelectron spectrum of a rare gas trimer by means of photoelectron-photoion coincidence techniques.

(8) This project produced two types of data on photoionization branching ratios and angular distributions for rare gas atoms. In one type of study, variations of these dynamical parameters within autoionizing resonances were measured. In the other type of study, the accurate, absolute β parameters for all the rare gases in the open continuum were measured as a point of reference for theory and spectrometer angular calibration in other labs.

(9) The mechanism of continuum-continuum coupling, leading to the transfer of shape resonant behavior between channels, was deduced by this project in a study on SF_6 and, subsequently, a study on N_2 confirmed a prediction of the effect in that system. These are initial studies of what is believed to be an important widespread phenomenon in molecular photoionization.

(10) This project developed a second generation triply differential photoelectron spectrometer which is the highest resolution and most sensitive electron spectrometer for use with synchrotron radiation.

(11) Finally, we have written several major book chapters giving detailed discussions of principles, bibliographies, and case studies of resonance processes in molecular photoionization.

IV. LIST OF PAPERS, ABSTRACTS OF CONTRIBUTED PAPERS, AND INVITED TALKS, COLLOQUIA, AND SEMINARS

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1. J. L. Dehmer and Dan Dill, "Shape Resonances in Molecular Photoionization," Plenary talk presented at Molecular Spectroscopy and Dynamics with Synchrotron Radiation-A European Workshop, Maria Laach, West Germany, September 29-October 1, 1980.

2. A. C. Parr, "Current Research at NBS Using Synchrotron Radiation at SURF-II," Invited talk presented at the Sixth Conference on the Application of Accelerators in Research and Industry, Denton, TX, November 3-5, 1980.

3. J. L. Dehmer, "Potpourri of Current and Future Studies of Molecular Photoionization-Synchrotron Radiation, Supersonic Jets, and Multiphoton Ionization," Chemistry Department Colloquium, Boston University, Boston, MA, 13 April 1981.

4. E. D. Poliakoff, "Two Novel Probes of Molecular Photoionization: Photoelectron-Photoion Coincidence Spectroscopy of Atomic Clusters and Fluorescence Polarization Analysis," Atomic and Molecular Science Seminar, Argonne National Laboratory, Argonne, Illinois, 6 May 1981.

5. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," Molecular Spectroscopy Division Seminar, National Bureau of Standards, Gaithersburg, MD, 21 May 1981.

6. E. D. Poliakoff, "Alignment of Molecular Ions Produced by Photoionization," Seminar on Collision Experiments in Their Theoretical Frame (Fano Workshop), The University of Chicago, Chicago, IL, 23 May 1981.

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16. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," Department of Physics Colloquium, University of Alabama, March 31, 1982.

17. J. L. Dehmer, "Molecular Photoionization Dynamics - Progress and Prospects," Physics Colloquium, University of Chicago, May 27, 1982.

18. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," California Institute of Technology, June 14, 1982.

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